



Autoencoders and Restricted Boltzmann Machines

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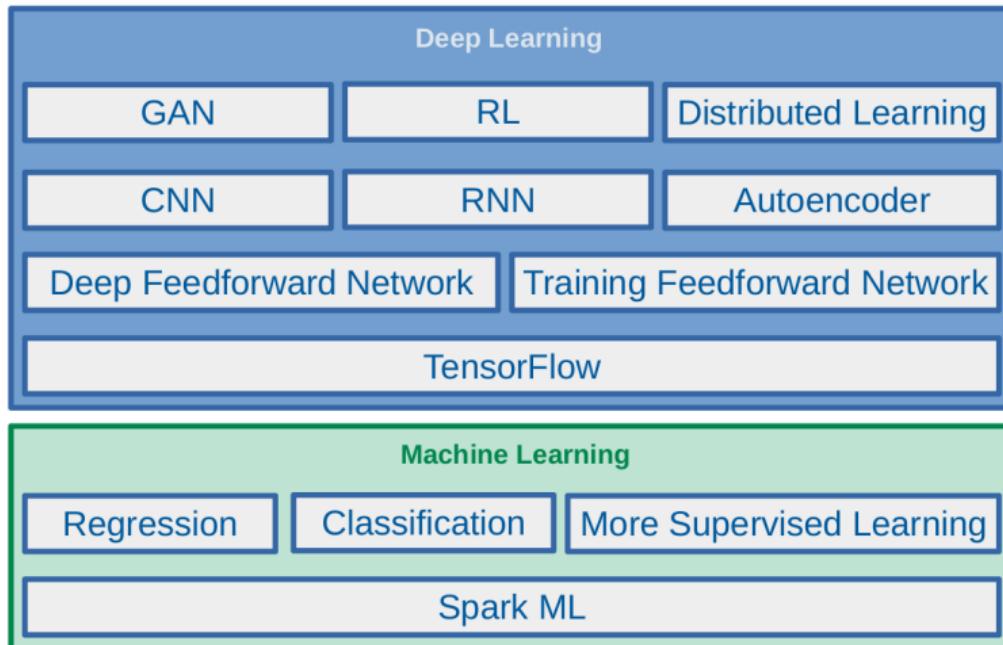


The Course Web Page

<https://id2223kth.github.io>

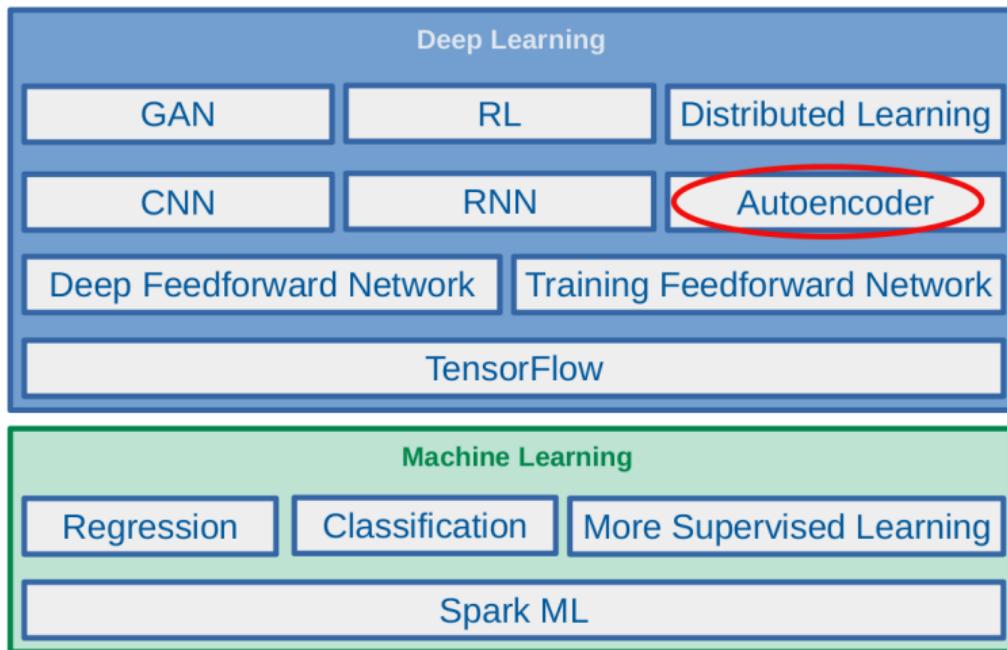


Where Are We?





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Let's Start With An Example



- ▶ Which of them is easier to memorize?

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- ▶ Seq1: 40, 27, 25, 36, 81, 57, 10, 73, 19, 68
- ▶ Seq2: 50, 25, 76, 38, 19, 58, 29, 88, 44, 22, 11, 34, 17, 52, 26, 13, 40, 20



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- ▶ But, Seq2 follows two simple rules:
 - Even numbers are followed by their half.
 - Odd numbers are followed by their triple plus one.



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 - Even numbers are followed by their half.
 - Odd numbers are followed by their triple plus one.
- ▶ You don't need pattern if you could quickly and easily memorize very long sequences
- ▶ But, it is hard to memorize long sequences that makes it useful to recognize patterns.



- ▶ 1970, W. Chase and H. Simon
- ▶ They observed that **expert chess players** were able to **memorize** the positions of **all** the pieces in a game by looking at the board for just **5 seconds**.



- ▶ This was only the case when the pieces were placed in **realistic positions**, not when the pieces were placed **randomly**.



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- ▶ Chess experts **don't have a much better memory** than you and I.
- ▶ They just see chess **patterns more easily** due to their **experience** with the game.
- ▶ **Patterns** helps them store information **efficiently**.

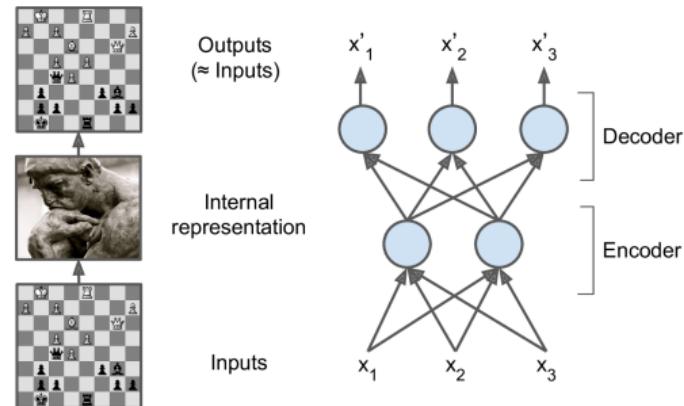




Autoencoders

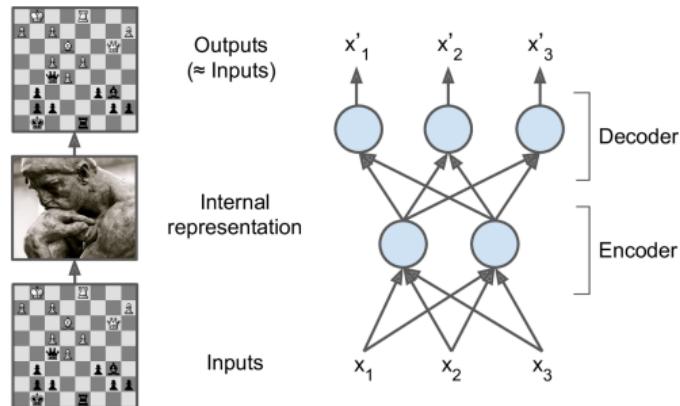
Autoencoders (1/5)

- ▶ Just like the chess players in this memory experiment.



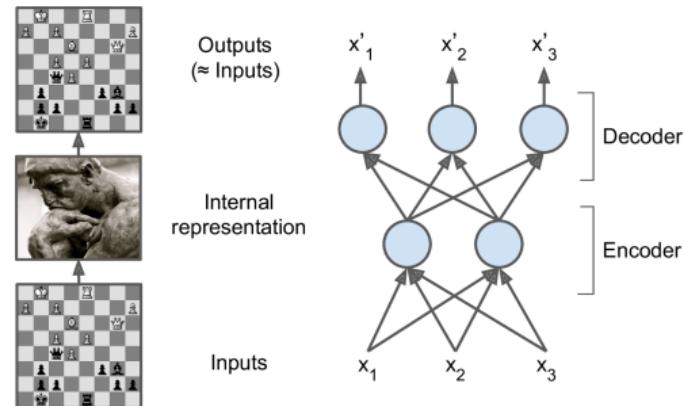
Autoencoders (1/5)

- ▶ Just like the chess players in this memory experiment.
- ▶ An **autoencoder** looks at the inputs, **converts** them to an efficient **internal representation**, and then **spits out** something that **looks very close to the inputs**.



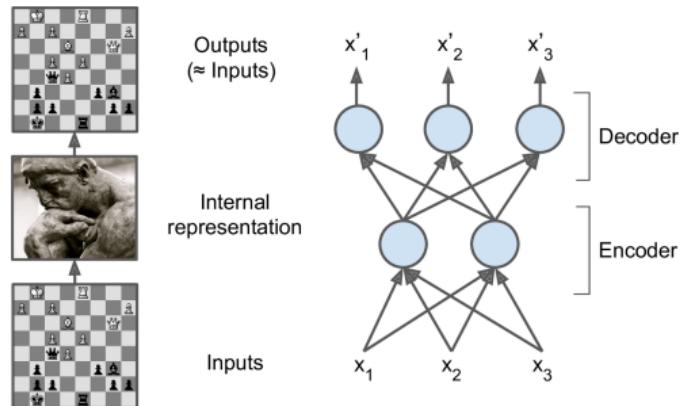
Autoencoders (2/5)

- ▶ The same architecture as a [Multi-Layer Perceptron \(MLP\)](#).



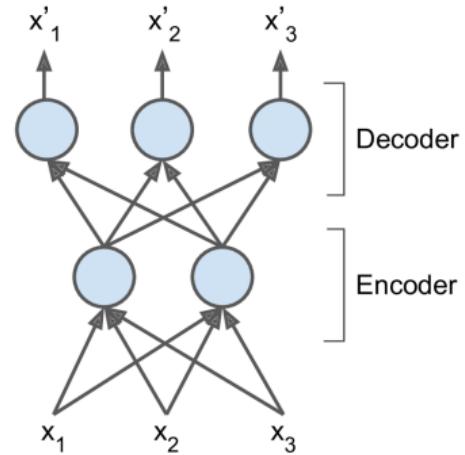
Autoencoders (2/5)

- ▶ The same architecture as a Multi-Layer Perceptron (MLP).
- ▶ Except that the number of neurons in the output layer must be **equal** to the **number of inputs**.



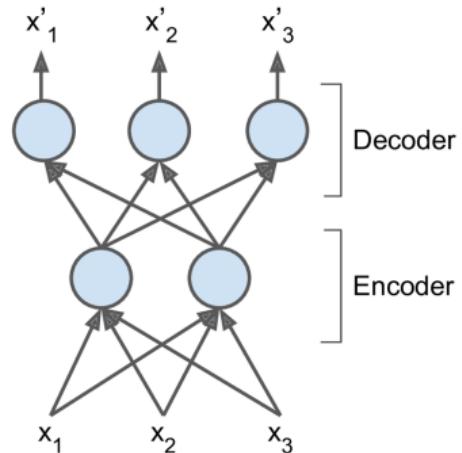
Autoencoders (3/5)

- ▶ An autoencoder is always composed of **two parts**.



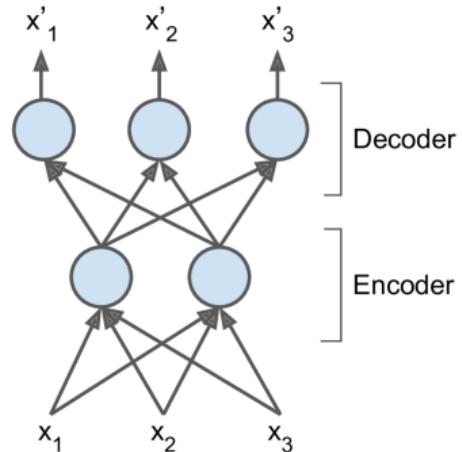
Autoencoders (3/5)

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- ▶ An **encoder (recognition network)**, $\mathbf{h} = f(\mathbf{x})$
Converts the **inputs** to an internal representation.



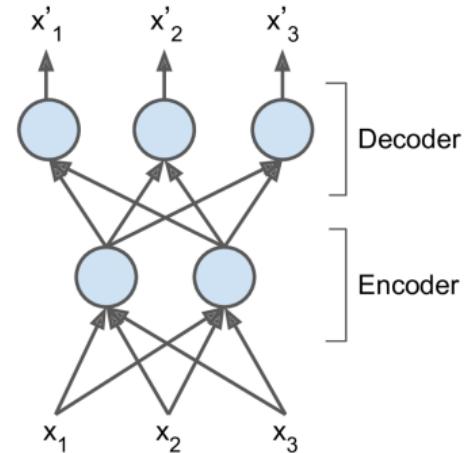
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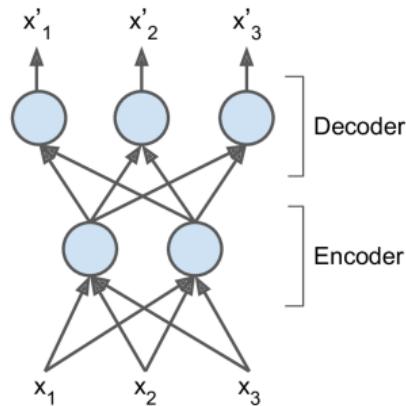
Autoencoders (3/5)

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- ▶ A **decoder (generative network)**, $\mathbf{r} = g(\mathbf{h})$
Converts the **internal representation** to the **outputs**.
- ▶ If an autoencoder learns to set $g(f(\mathbf{x})) = \mathbf{x}$ everywhere, it is **not especially useful**, **why?**



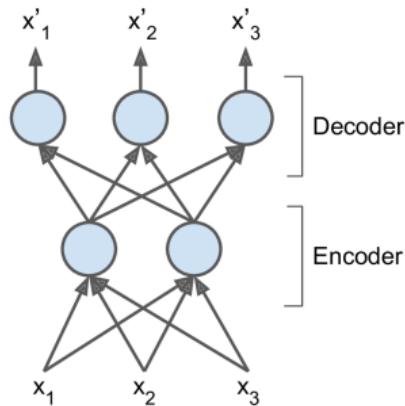
Autoencoders (4/5)

- ▶ Autoencoders are designed to be **unable** to learn to copy perfectly.



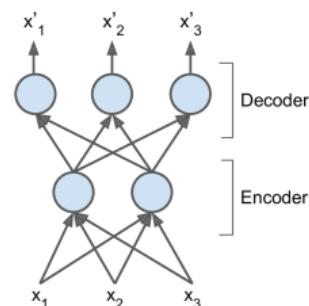
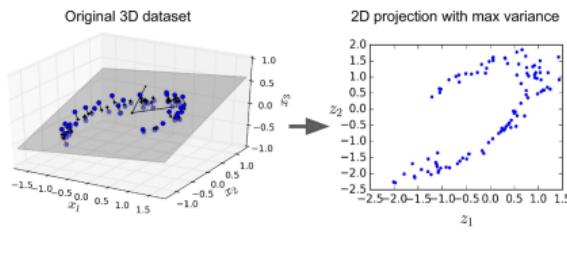
Autoencoders (4/5)

- ▶ Autoencoders are designed to be **unable** to learn to copy perfectly.
- ▶ The models are forced to **prioritize which aspects of the input** should be copied, they often learn **useful properties** of the data.



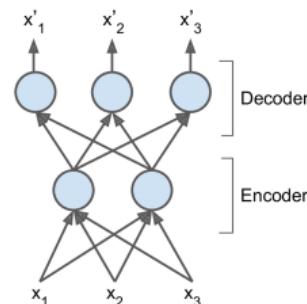
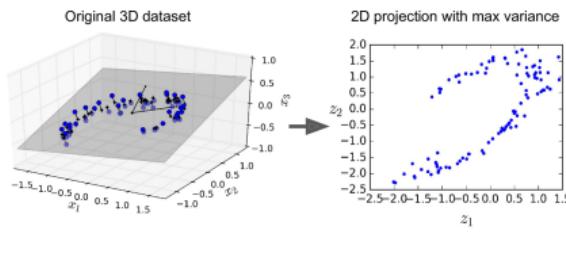
Autoencoders (5/5)

- ▶ Autoencoders are neural networks capable of learning efficient representations of the input data (called codings) without any supervision.



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- ▶ Autoencoders are neural networks capable of learning efficient representations of the input data (called codings) without any supervision.
- ▶ Dimension reduction: these codings typically have a much lower dimensionality than the input data.





Different Types of Autoencoders

- ▶ Stacked autoencoders
- ▶ Denoising autoencoders
- ▶ Sparse autoencoders
- ▶ Variational autoencoders

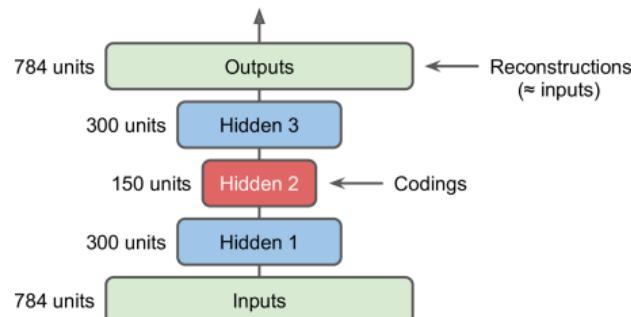


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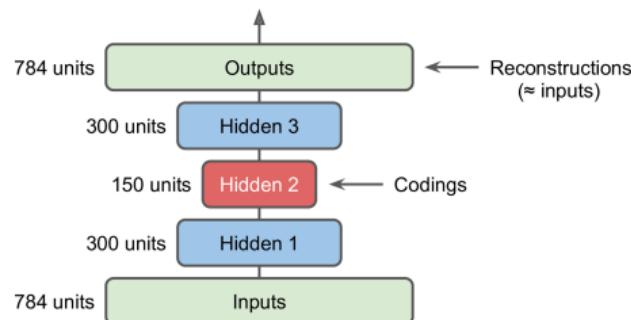
Stacked Autoencoders (1/3)

- ▶ **Stacked autoencoder**: autoencoders with **multiple hidden layers**.



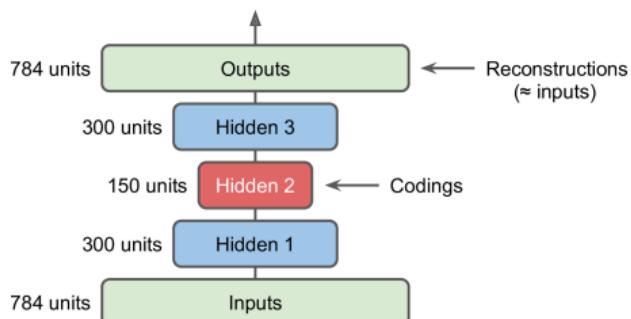
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- ▶ **Stacked autoencoder**: autoencoders with **multiple hidden layers**.
- ▶ Adding **more layers** helps the autoencoder learn more **complex codings**.



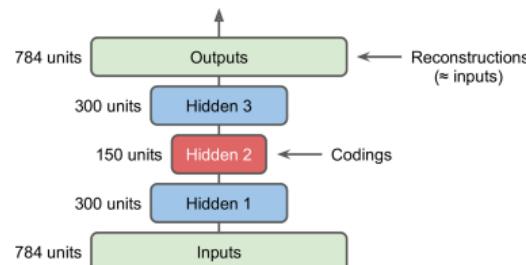
Stacked Autoencoders (1/3)

- ▶ **Stacked autoencoder**: autoencoders with **multiple hidden layers**.
- ▶ Adding **more layers** helps the autoencoder learn more **complex codings**.
- ▶ The architecture is typically **symmetrical** with regards to the **central hidden layer**.



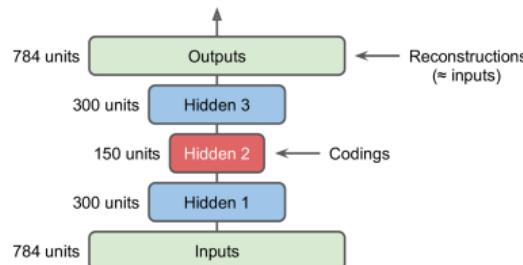
Stacked Autoencoders (2/3)

- In a symmetric architecture, we can **tie the weights** of the **decoder layers** to the weights of the **encoder layers**.



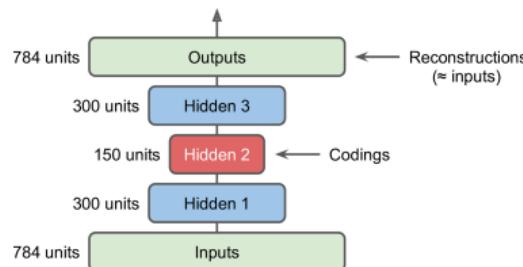
Stacked Autoencoders (2/3)

- ▶ In a symmetric architecture, we can **tie the weights** of the **decoder layers** to the weights of the **encoder layers**.
- ▶ In a network with **N** layers, the **decoder layer weights** can be defined as $w_{N-1+1} = w_1^T$, with $l = 1, 2, \dots, \frac{N}{2}$.



Stacked Autoencoders (2/3)

- ▶ In a symmetric architecture, we can **tie the weights** of the **decoder layers** to the weights of the **encoder layers**.
- ▶ In a network with **N** layers, the **decoder layer weights** can be defined as $w_{N-1+1} = w_1^T$, with $l = 1, 2, \dots, \frac{N}{2}$.
- ▶ This **halves** the **number of weights** in the model, **speeding up training** and **limiting the risk of overfitting**.





Stacked Autoencoders (3/3)

```
stacked_encoder = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.Dense(100, activation="relu"),
    keras.layers.Dense(30, activation="relu"),
])
stacked_decoder = keras.models.Sequential([
    keras.layers.Dense(100, activation="relu", input_shape=[30]),
    keras.layers.Dense(28 * 28, activation="sigmoid"),
    keras.layers.Reshape([28, 28])
])
model = keras.models.Sequential([stacked_encoder, stacked_decoder])
```

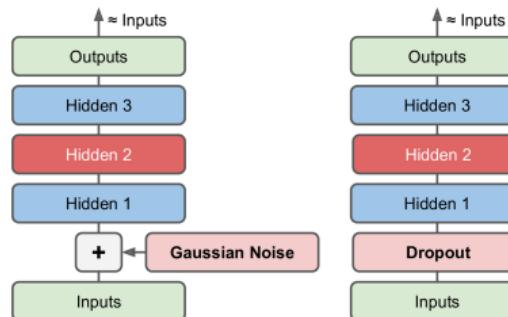


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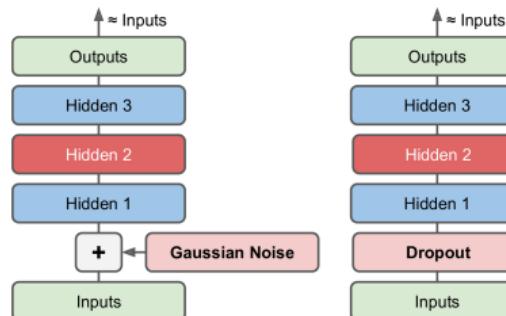
Denoising Autoencoders (1/4)

- ▶ One way to force the autoencoder to **learn useful features** is to **add noise** to its **inputs**, training it to **recover the original noise-free inputs**.



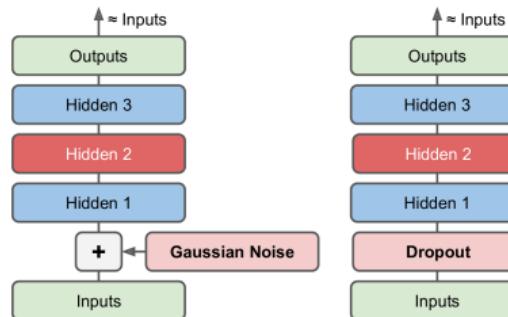
Denoising Autoencoders (1/4)

- ▶ One way to force the autoencoder to **learn useful features** is to **add noise** to its **inputs**, training it to **recover the original noise-free inputs**.
- ▶ This prevents the autoencoder from **trivially copying** its **inputs** to its **outputs**, so it ends up having to find patterns in the data.



Denoising Autoencoders (2/4)

- The noise can be pure Gaussian noise added to the inputs, or it can be randomly switched off inputs, just like in dropout.





Denoising Autoencoders (3/4)

```
denoising_encoder = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.Dropout(0.5),
    keras.layers.Dense(100, activation="relu"),
    keras.layers.Dense(30, activation="relu")
])
denoising_decoder = keras.models.Sequential([
    keras.layers.Dense(100, activation="relu", input_shape=[30]),
    keras.layers.Dense(28 * 28, activation="sigmoid"),
    keras.layers.Reshape([28, 28])
])
model = keras.models.Sequential([denoising_encoder, denoising_decoder])
```



Denoising Autoencoders (4/4)

```
denoising_encoder = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.GaussianNoise(0.2),
    keras.layers.Dense(100, activation="relu"),
    keras.layers.Dense(30, activation="relu")
])
denoising_decoder = keras.models.Sequential([
    keras.layers.Dense(100, activation="relu", input_shape=[30]),
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])
model = keras.models.Sequential([denoising_encoder, denoising_decoder])
```



Different Types of Autoencoders

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- ▶ **Sparse autoencoders**
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Sparse Autoencoders (1/2)

- ▶ Adding an appropriate term to the **cost function** to push the autoencoder to **reducing** the number of **active neurons** in the **coding layer**.



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Sparse Autoencoders (1/2)

- ▶ Adding an appropriate term to the **cost function** to push the autoencoder to **reducing** the number of **active neurons** in the **coding layer**.
- ▶ This forces the autoencoder to represent each input as a combination of a **small number of activations**.
- ▶ As a result, **each neuron** in the **coding layer** typically ends up representing a **useful feature**.



Sparse Autoencoders (2/2)

```
sparse_l1_encoder = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.Dense(100, activation="selu"),
    keras.layers.Dense(300, activation="sigmoid", activity_regularizer=keras.regularizers.l1(1e-3))
])

sparse_l1_decoder = keras.models.Sequential([
    keras.layers.Dense(100, activation="selu", input_shape=[300]),
    keras.layers.Dense(28 * 28, activation="sigmoid"),
    keras.layers.Reshape([28, 28])
])

model = keras.models.Sequential([sparse_l1_encoder, sparse_l1_decoder])
```



Different Types of Autoencoders

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Variational Autoencoders (1/6)

- ▶ Variational autoencoders are probabilistic autoencoders.



Variational Autoencoders (1/6)

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- ▶ Their outputs are partly determined by chance, even after training.
 - As opposed to denoising autoencoders, which use randomness only during training.

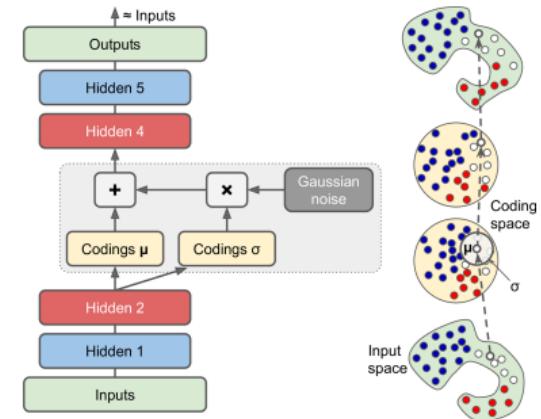


Variational Autoencoders (1/6)

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- ▶ Their outputs are partly determined by chance, even after training.
 - As opposed to denoising autoencoders, which use randomness only during training.
- ▶ They are generative autoencoders, meaning that they can generate new instances that look like they were sampled from the training set.

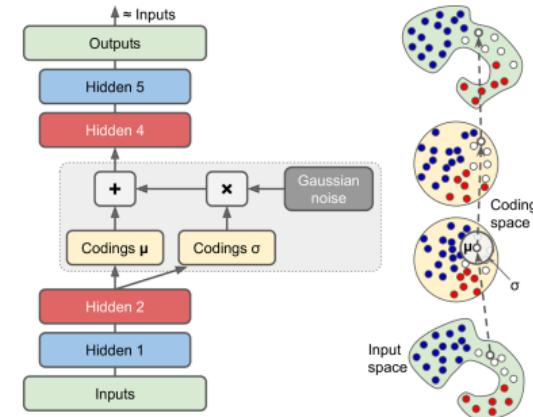
Variational Autoencoders (2/6)

- ▶ Instead of directly producing a coding for a given input, the **encoder** produces a **mean coding μ** and a **standard deviation σ** .



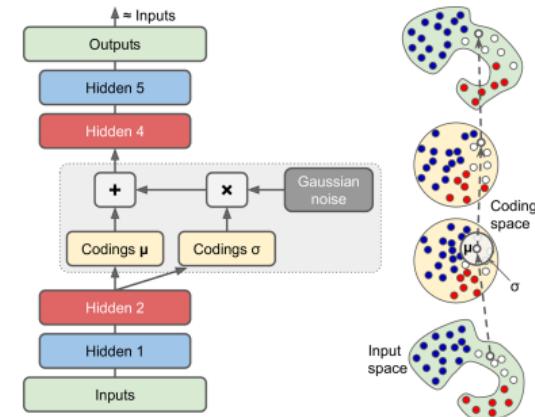
Variational Autoencoders (2/6)

- ▶ Instead of directly producing a coding for a given input, the **encoder** produces a **mean coding μ** and a **standard deviation σ** .
- ▶ The **actual coding** is then **sampled randomly** from a **Gaussian distribution** with mean μ and standard deviation σ .



Variational Autoencoders (2/6)

- ▶ Instead of directly producing a coding for a given input, the **encoder** produces a **mean coding μ** and a **standard deviation σ** .
- ▶ The **actual coding** is then **sampled randomly** from a **Gaussian distribution** with mean μ and **standard deviation σ** .
- ▶ After that the **decoder** just **decodes** the sampled coding normally.





Variational Autoencoders (3/6)

- ▶ The **cost function** is composed of **two parts**.



Variational Autoencoders (3/6)

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 - Pushes the autoencoder to **reproduce its inputs**.
 - Using **cross-entropy**.



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 - Pushes the autoencoder to have **codings** that look as though they were sampled from a simple **Gaussian distribution**.



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 - Using the **KL divergence** between the **target distribution** (the Gaussian distribution) and the **actual distribution** of the codings.



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 - Pushes the autoencoder to **reproduce its inputs**.
 - Using **cross-entropy**.
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 - Pushes the autoencoder to have **codings** that look as though they were sampled from a **simple Gaussian distribution**.
 - Using the **KL divergence** between the **target distribution** (the Gaussian distribution) and the **actual distribution** of the codings.
 - $$\text{latent_loss} = -\frac{1}{2} \sum_1^K (1 + \log(\sigma_i^2) - \sigma_i^2 - \mu_i^2)$$



Variational Autoencoders (4/6)

► Encoder part

```
inputs = keras.layers.Input(shape=[28, 28])
z = keras.layers.Flatten()(inputs)
z = keras.layers.Dense(150, activation="relu")(z)
z = keras.layers.Dense(100, activation="relu")(z)
codings_mean = keras.layers.Dense(10)(z)
codings_log_var = keras.layers.Dense(10)(z)
codings = Sampling()([codings_mean, codings_log_var]) # normal distribution
variational_encoder = keras.models.Model(inputs=[inputs], outputs=[codings])
```



Variational Autoencoders (5/6)

► Decoder part

```
decoder_inputs = keras.layers.Input(shape=[codings_size])
x = keras.layers.Dense(100, activation="relu")(decoder_inputs)
x = keras.layers.Dense(150, activation="relu")(x)
x = keras.layers.Dense(28 * 28, activation="sigmoid")(x)
outputs = keras.layers.Reshape([28, 28])(x)
variational_decoder = keras.models.Model(inputs=[decoder_inputs], outputs=[outputs])
```



Variational Autoencoders (6/6)

```
codings = variational_encoder(inputs)
reconstructions = variational_decoder(codings)
model = keras.models.Model(inputs=[inputs], outputs=[reconstructions])

latent_loss = -0.5 * K.sum(1 + codings_log_var - K.exp(codings_log_var)
                           - K.square(codings_mean), axis=-1)
model.add_loss(K.mean(latent_loss) / 784.)
```

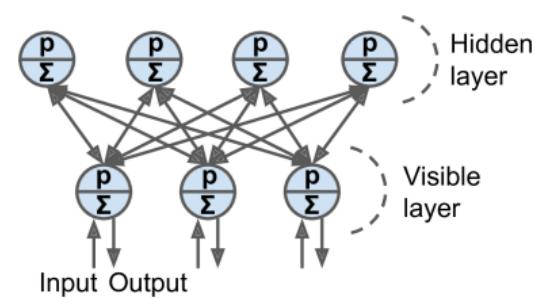




Restricted Boltzmann Machines

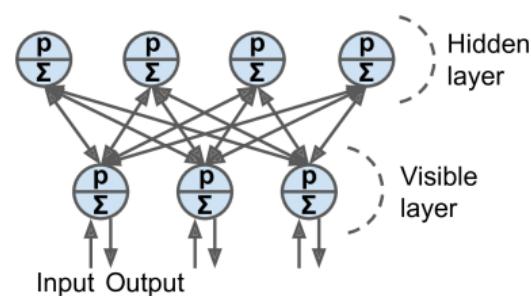
Restricted Boltzmann Machines

- A Restricted Boltzmann Machine (RBM) is a stochastic neural network.



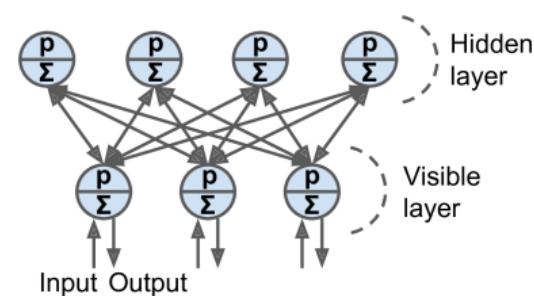
Restricted Boltzmann Machines

- ▶ A Restricted Boltzmann Machine (RBM) is a stochastic neural network.
- ▶ Stochastic meaning these activations have a probabilistic element, instead of deterministic functions, e.g., logistic or ReLU.



Restricted Boltzmann Machines

- ▶ A Restricted Boltzmann Machine (RBM) is a stochastic neural network.
- ▶ Stochastic meaning these activations have a probabilistic element, instead of deterministic functions, e.g., logistic or ReLU.
- ▶ The neurons form a bipartite graph:
 - One visible layer and one hidden layer.
 - A symmetric connection between the two layers.
 - There are no connections between neurons within a layer.





Let's Start With An Example

RBM Example (1/10)

- We have a set of **six movies**, and we ask users to tell us which ones **they want to watch**.



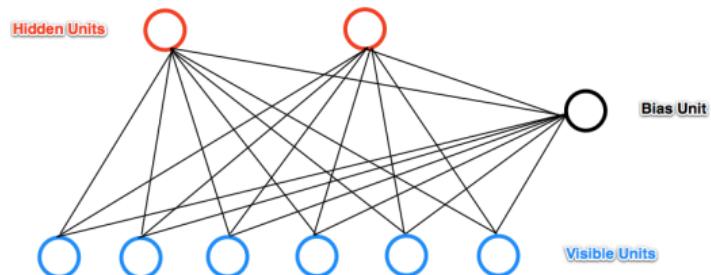
RBM Example (1/10)

- ▶ We have a set of **six movies**, and we ask users to tell us which ones **they want to watch**.
- ▶ We want to learn two **latent neurons (hidden neurons)** underlying movie preferences, e.g., **SF/fantasy** and **Oscar winners**



RBM Example (2/10)

- ▶ Our RBM would look like the following.



RBM Example (3/10)

- ▶ Alice: (HP=1, Avatar=1, LOTR=1, Glad=0, Titan=0, Sep=0), Big SF fan.



RBM Example (3/10)

- ▶ Alice: (HP=1, Avatar=1, LOTR=1, Glad=0, Titan=0, Sep=0), Big SF fan.
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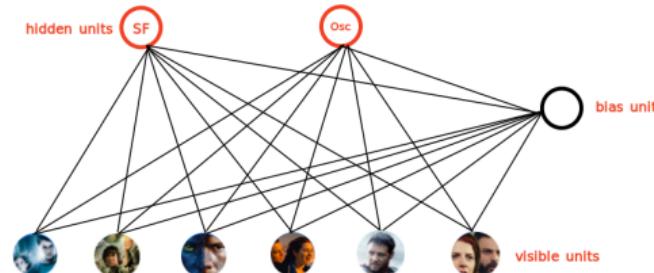
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RBM Example (3/10)

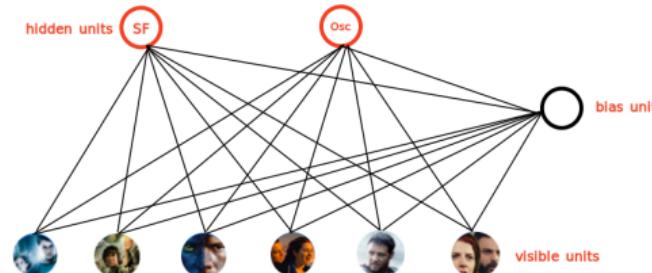
- ▶ Assume the given input x_i is the 0 or 1 for each visible neuron v_i .
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RBM Example (3/10)

- ▶ Assume the given input x_i is the 0 or 1 for each visible neuron v_i .
 - 1: like a movie, and 0: dislike a movie
- ▶ Compute the activation energy at hidden neuron h_j :

$$a(h_j) = \sum_i w_{ij} v_i$$

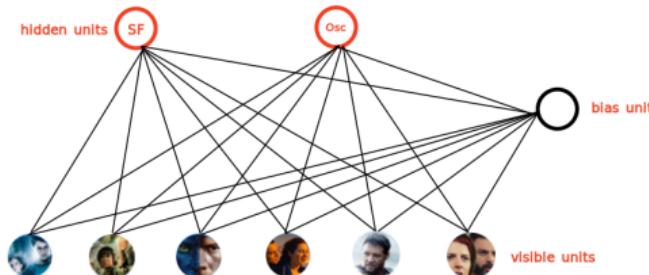


RBM Example (4/10)

- ▶ For each hidden neuron h_j , we compute the probability $p(h_j)$.

$$a(h_j) = \sum_i w_{ij} v_i$$

$$p(h_j) = \text{sigmoid}(a(h_j)) = \frac{1}{1 + e^{-a(h_j)}}$$



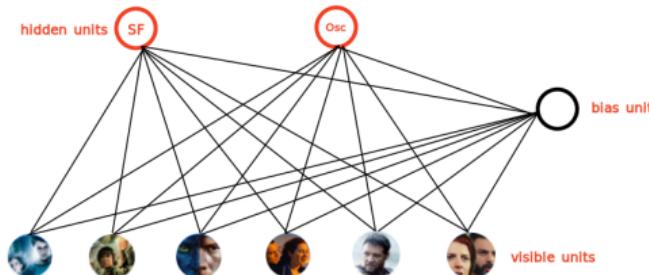
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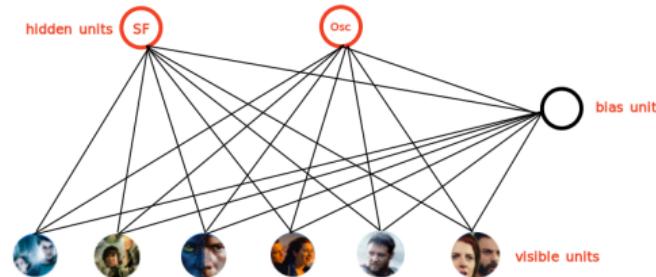
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- ▶ We turn on the hidden neuron h_j with the probability $p(h_j)$, and turn it off with probability $1 - p(h_j)$.



RBM Example (5/10)

- ▶ Declaring that you like Harry Potter, Avatar, and LOTR, doesn't guarantee that the SF/fantasy hidden neuron will turn on.



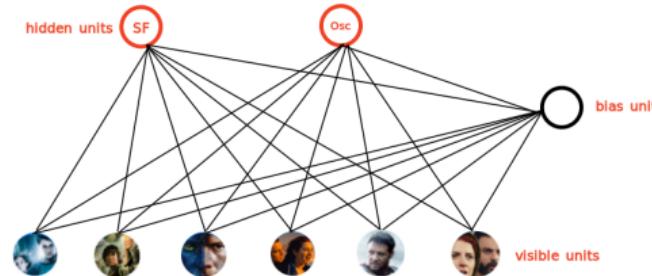
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- ▶ But it will turn on with a high probability.
 - In reality, if you want to watch all three of those movies makes us highly suspect you like SF/fantasy in general.
 - But there's a small chance you like them for other reasons.





RBM Example (6/10)

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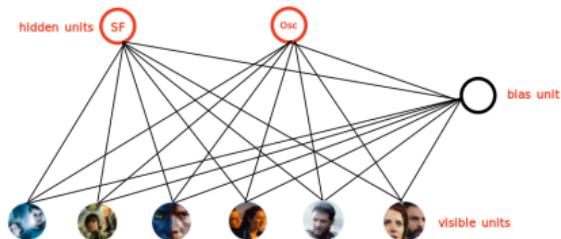
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- ▶ Being on the **SF/fantasy** neuron **doesn't guarantee** that we'll always recommend all three of **Harry Potter**, **Avatar**, and **LOTR**.
 - For example **not everyone** who likes science fiction liked Avatar.

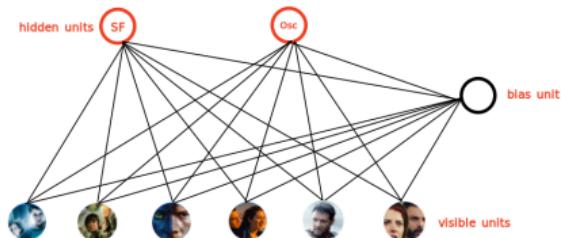
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- ▶ Assume, as an input we have a bunch of **binary vectors x** with **six elements** corresponding to a **user's movie preferences**.
- ▶ We do the **following steps** in each **epoch**:
- ▶ 1. Take a **training instance x** and set the **states** of the **visible neurons** to these preferences.



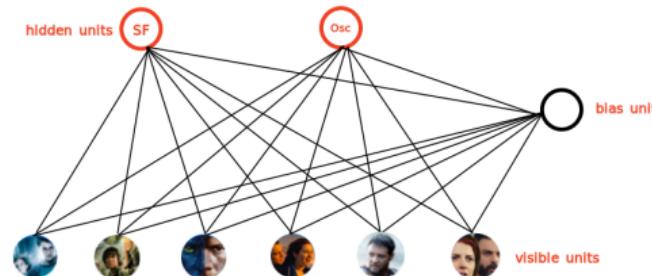
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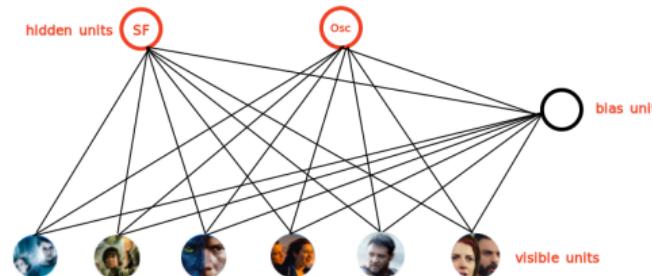
- ▶ 2. Update the **states** of the **hidden neurons**.

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- ▶ 3. For each edge e_{ij} , compute **positive**(e_{ij}) = $v_i \times h_j$
 - I.e., for each **pair of neurons**, measure whether they are **both on**.



RBM Example (9/10)

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 - We denote the updated visible neurons with v'_i .
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- ▶ 6. For each edge e_{ij} , compute **negative**(e_{ij}) = $v'_i \times h'_j$



RBM Example (10/10)

- ▶ 7. Update the weight of each edge e_{ij} .

$$w_{ij} = w_{ij} + \eta(\text{positive}(e_{ij}) - \text{negative}(e_{ij}))$$



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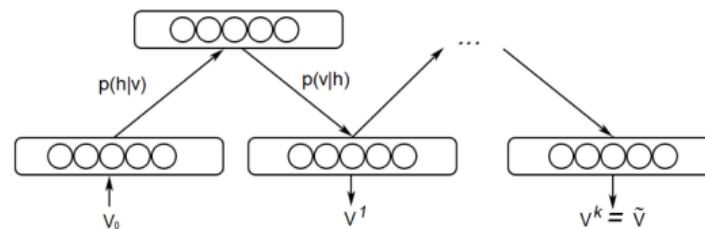
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- ▶ 8. Repeat over all training examples.
- ▶ 9. Continue until the error between the training examples and their reconstructions falls below some threshold or we reach some maximum number of epochs.



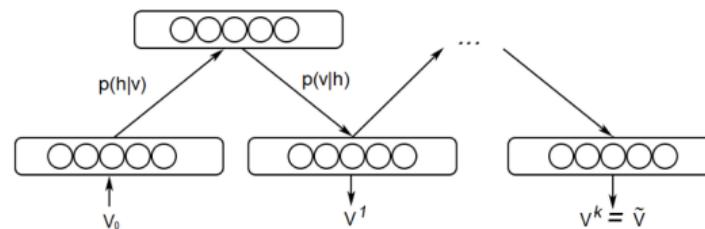
RBM Training (1/2)

- ▶ Step 1, Gibbs sampling: what we have done in steps 1-6.



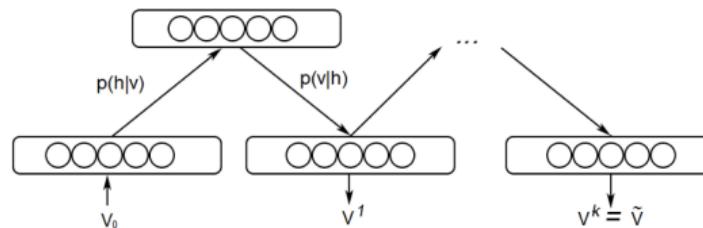
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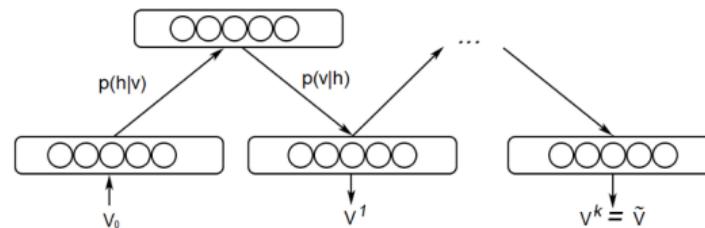
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- ▶ This process is repeated k times.





RBM Training (2/2)

- ▶ Step 2, **contrastive divergence**: what we have done in step 7.
 - Just a fancy name for **approximate gradient descent**.

$$\mathbf{w} = \mathbf{w} + \eta(\text{positive}(\mathbf{e}) - \text{negative}(\mathbf{e}))$$



More Details about RBM



Energy-based Model (1/3)

- ▶ Energy a quantitative property of physics.

Energy-based Model (1/3)

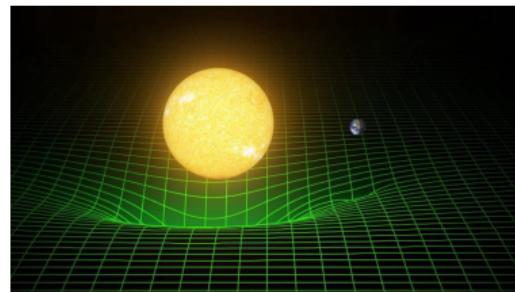
► Energy a quantitative property of physics.

- E.g., gravitational energy describes the potential energy a body with mass has in relation to another massive object due to gravity.



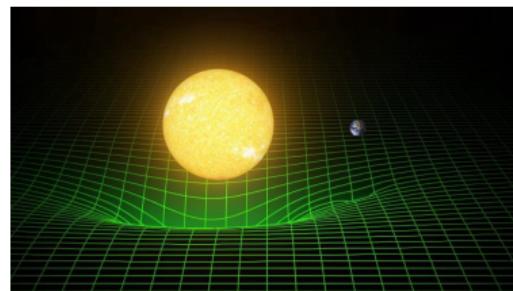
Energy-based Model (2/3)

- ▶ One purpose of deep learning models is to **encode dependencies between variables**.



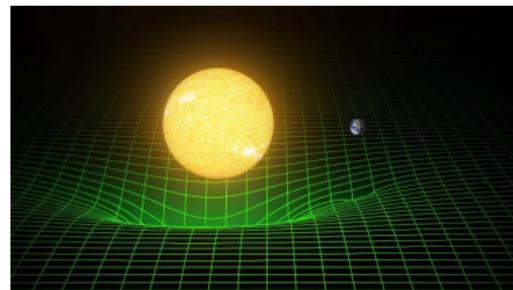
Energy-based Model (2/3)

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- ▶ The capturing of **dependencies** happen through associating of a **scalar energy** to each **state of the variables**.
 - Serves as a **measure of compatibility**.



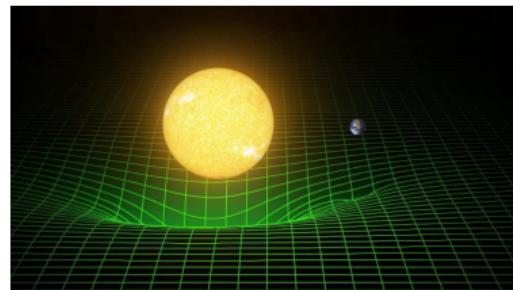
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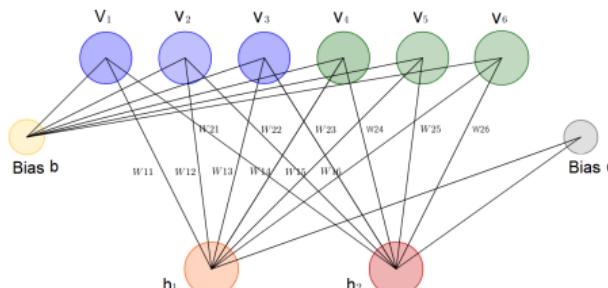
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- ▶ A **high energy** means a **bad compatibility**.
- ▶ An **energy based model** tries always to **minimize** a predefined energy function.



Energy-based Model (3/3)

- ▶ The **energy function** for the RBMs is defined as:

$$E(\mathbf{v}, \mathbf{h}) = -\left(\sum_{ij} w_{ij} v_i h_j + \sum_i b_i v_i + \sum_j c_j h_j\right)$$

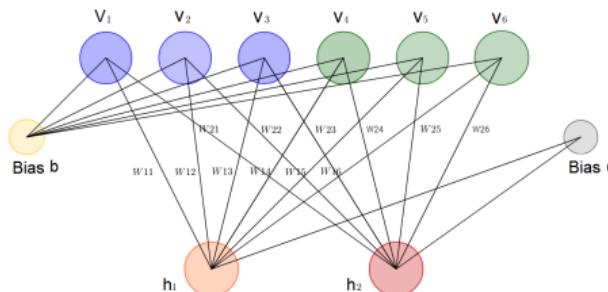


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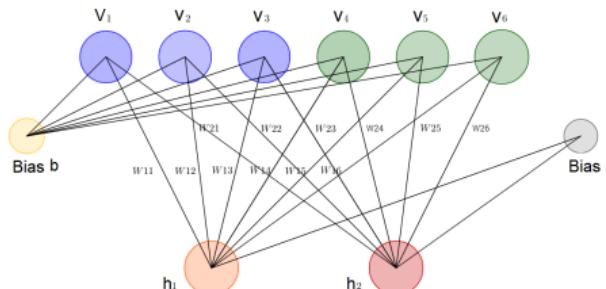


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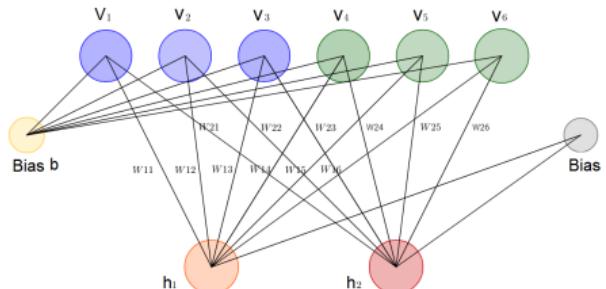


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- ▶ **b** and **c** are the **biases** of the visible and hidden layers, respectively.





RBM is a Probabilistic Model (1/2)

- ▶ The probability of a certain state of v and h :

$$p(v, h) = \frac{e^{-E(v, h)}}{\sum_{v, h} e^{-E(v, h)}}$$



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- ▶ In physics, the joint distribution $p(v, h)$ is known as the **Boltzmann Distribution** or **Gibbs Distribution**.
- ▶ At each point in time the RBM is in a certain state.
 - The state refers to the values of neurons in the visible and hidden layers v and h .



RBM is a Probabilistic Model (2/2)

- ▶ It is **difficult** to calculate the **joint probability** due to the **huge number of possible combination** of **v** and **h**.

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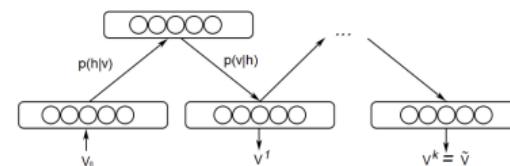
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- ▶ Much easier is the calculation of the **conditional probabilities** of state **h** given the state **v** and vice versa (**Gibbs sampling**)

$$p(h|v) = \prod_i p(h_i|v)$$

$$p(v|h) = \prod_j p(v_j|h)$$





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$$p(\mathbf{v}|\mathbf{h}) = \frac{\sum_{\mathbf{h}} e^{-E(\mathbf{v}, \mathbf{h})}}{\sum_{\mathbf{v}, \mathbf{h}} e^{-E(\mathbf{v}, \mathbf{h})}}$$

- ▶ Use the maximum-likelihood estimation.
- ▶ For a model of the form $p(\mathbf{v})$ with parameters \mathbf{w} , the log-likelihood given a single training example \mathbf{v} is:

$$\log p(\mathbf{v}|\mathbf{h}) = \log \frac{\sum_{\mathbf{h}} e^{-E(\mathbf{v}, \mathbf{h})}}{\sum_{\mathbf{v}, \mathbf{h}} e^{-E(\mathbf{v}, \mathbf{h})}} = \log \sum_{\mathbf{h}} e^{-E(\mathbf{v}, \mathbf{h})} - \log \sum_{\mathbf{v}, \mathbf{h}} e^{-E(\mathbf{v}, \mathbf{h})}$$

Learning in Boltzmann Machines (2/2)

- ▶ The **log-likelihood gradients** for an RBM with **binary units**:

$$\frac{\partial \log p(\mathbf{v}|\mathbf{h})}{\partial w_{ij}} = \text{positive}(e_{ij}) - \text{negative}(e_{ij})$$

Learning in Boltzmann Machines (2/2)

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- ▶ Then, we can **update** the weight **w** as follows:

$$w_{ij}^{(\text{next})} = w_{ij} + \eta(\text{positive}(e_{ij}) - \text{negative}(e_{ij}))$$



IT'S OVER

IT'S FINALLY OVER

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Summary



Summary

- ▶ Autoencoders
 - Stacked autoencoders
 - Denoising autoencoders
 - Variational autoencoders
- ▶ Restricted Boltzmann Machine
 - Gibbs sampling
 - Contrastive divergence



Reference

- ▶ Ian Goodfellow et al., Deep Learning (Ch. 14, 20)
- ▶ Aurélien Géron, Hands-On Machine Learning (Ch. 17)



Questions?